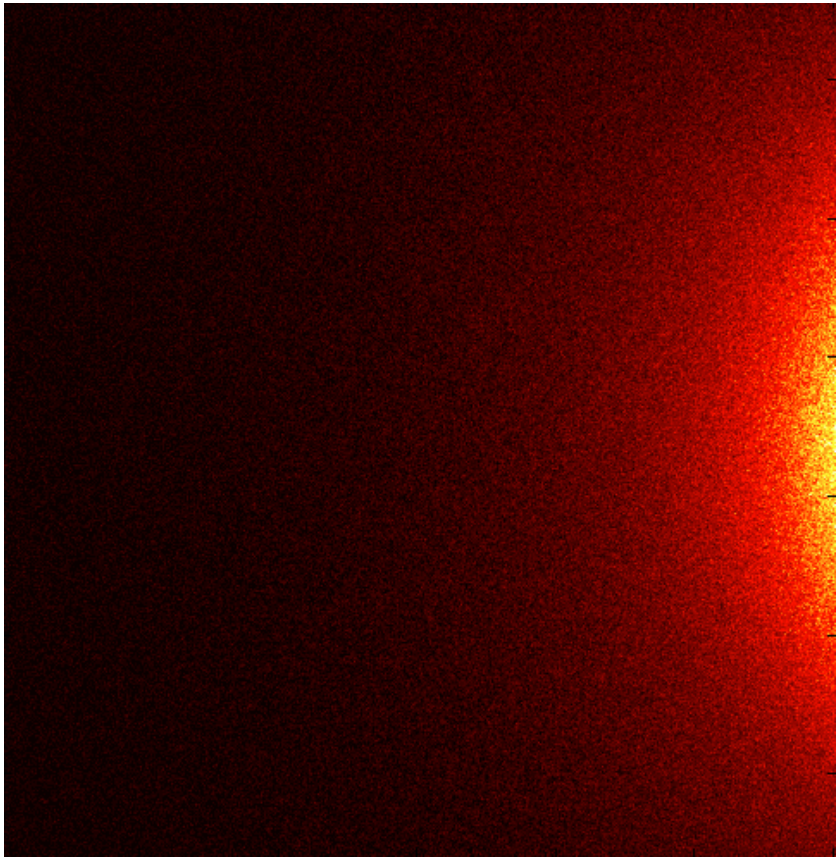
Analysis of LCLS Visibility Tests



The Visibility Tests

- Systematic variation in the number of x-ray pulses (“shots”) that hit the sample in a single exposure (“frame”).
- Two samples were studied: gold nanoparticles (~10 nm) in polystyrene 42k @ 170 C (Au-NPs), and dry silica spheres (~150 nm) at room temperature (Si).
- This was done both to measure the contrast within a single frame, and to compare potential differences between the Au-NPs and a (ostensibly) static sample.

Some Details

- The shots/frame were 2, 5, 10, 20, 100
- For the following analysis, I worked with a region where average intensity was high, in an annulus centered at Q=0.05 Å^-1, with a width of ΔQ/Q = 10%.
- An averaged dark image was subtracted from all frames, and any pixel values <25 were replaced with zeros (typical adu = 1640).

V2 & Contrast

- Typically, when someone speaks about the contrast of a speckle pattern, they are referring to the quantity:

$$C = \sigma_I / \bar{I}$$

- In speckle variance/visibility spectroscopy (SVS), the quantity of interest is:

$$V_2 = Var(I)/\bar{I}^2 = C^2$$

V2 & dynamics (SVS)

- If one merges together snapshots of a moving speckle pattern, the contrast of the combined image will decrease.
- If sample dynamics are the cause, V2 is related to them in an analytic way:

$$V_2(T) = \frac{1}{\beta}\left[\frac{<I^2>_T}{<I>^2} - 1\right] = \int_0^T 2(1 - t/T)[g_1(t)]^2 dt/T$$

- For example,

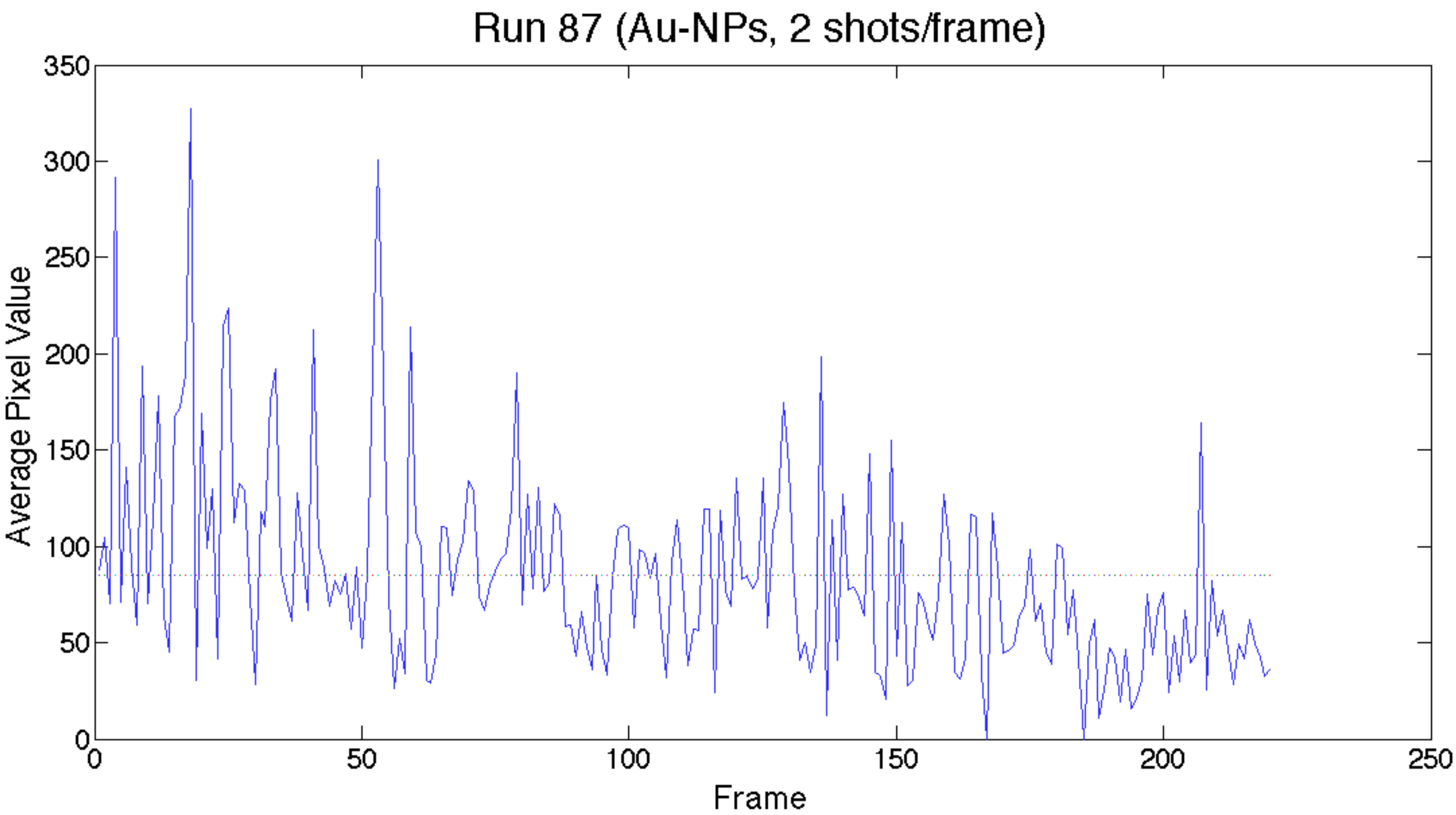
$$g_1(\tau) = e^{-\Gamma\tau} => V_2 = \frac{e^{-2\Gamma\tau} - 1 + 2\Gamma\tau}{2(\Gamma\tau)^2}$$

(Bandyopadhyay, et. al.)

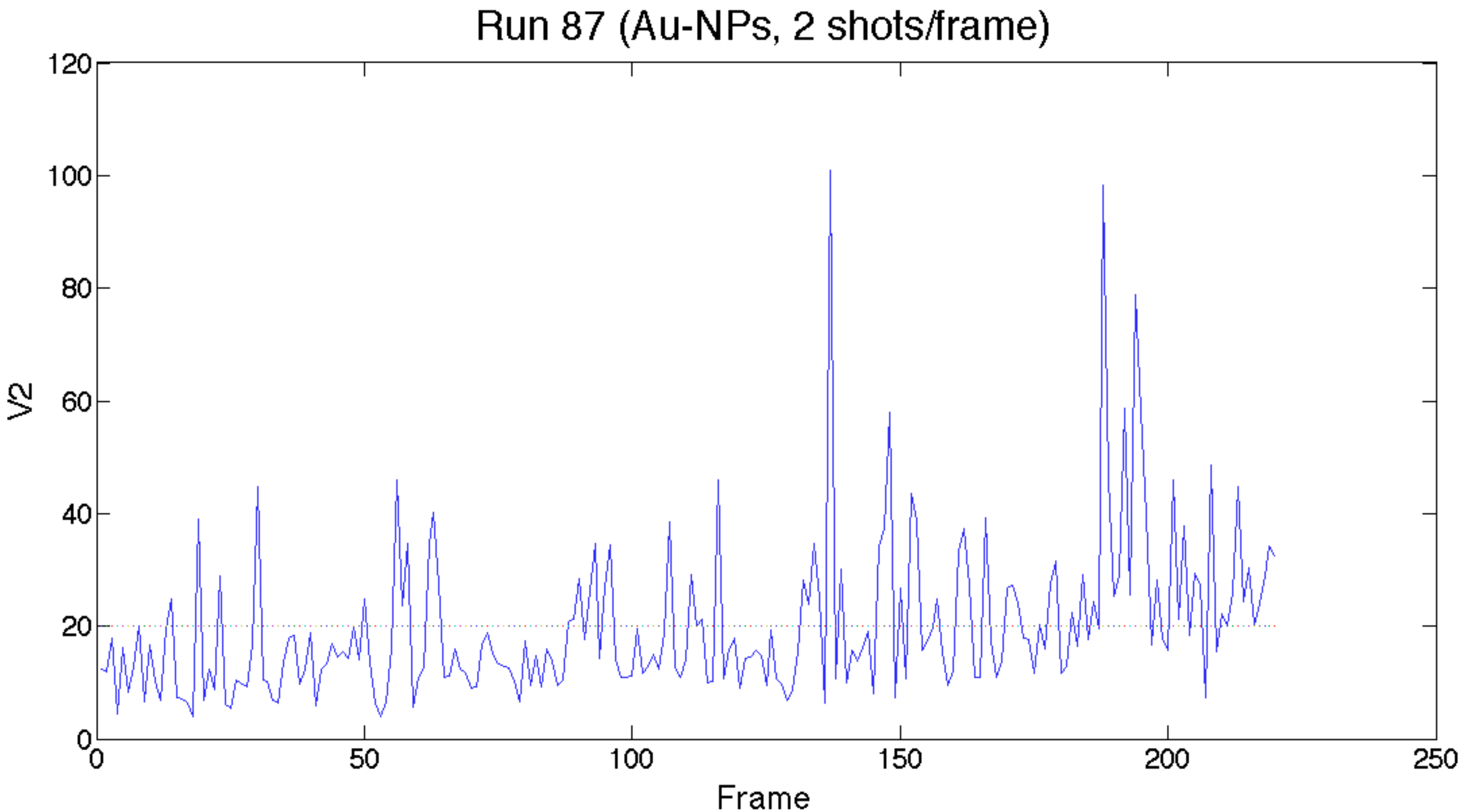
V2 and Poisson noise

- A perfectly coherent beam and sufficient photons produce an exponential distribution of speckle intensity (see Goodman's books), which implies C=V2=1.
- However, when there are few photons, the probability of getting a photon count at a given pixel should follow a Poisson distribution (so-called "shot noise").
- For pure Poisson noise, one finds that V2=1/p, where p is the mean # of counts per pixel. Clearly, this becomes large as p --> 0.

At LCLS, the intensity varies greatly from frame to frame…

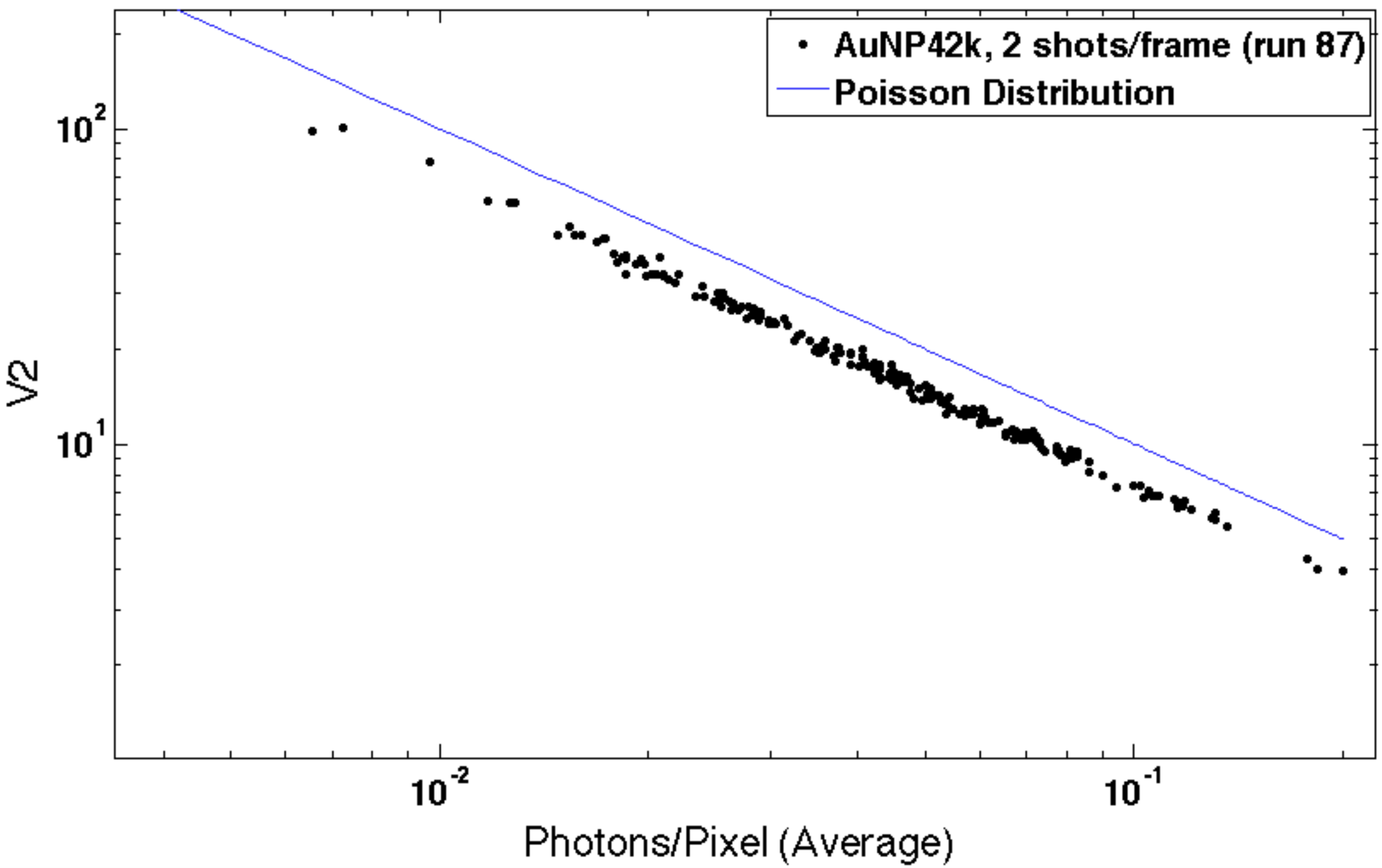


As does V2…



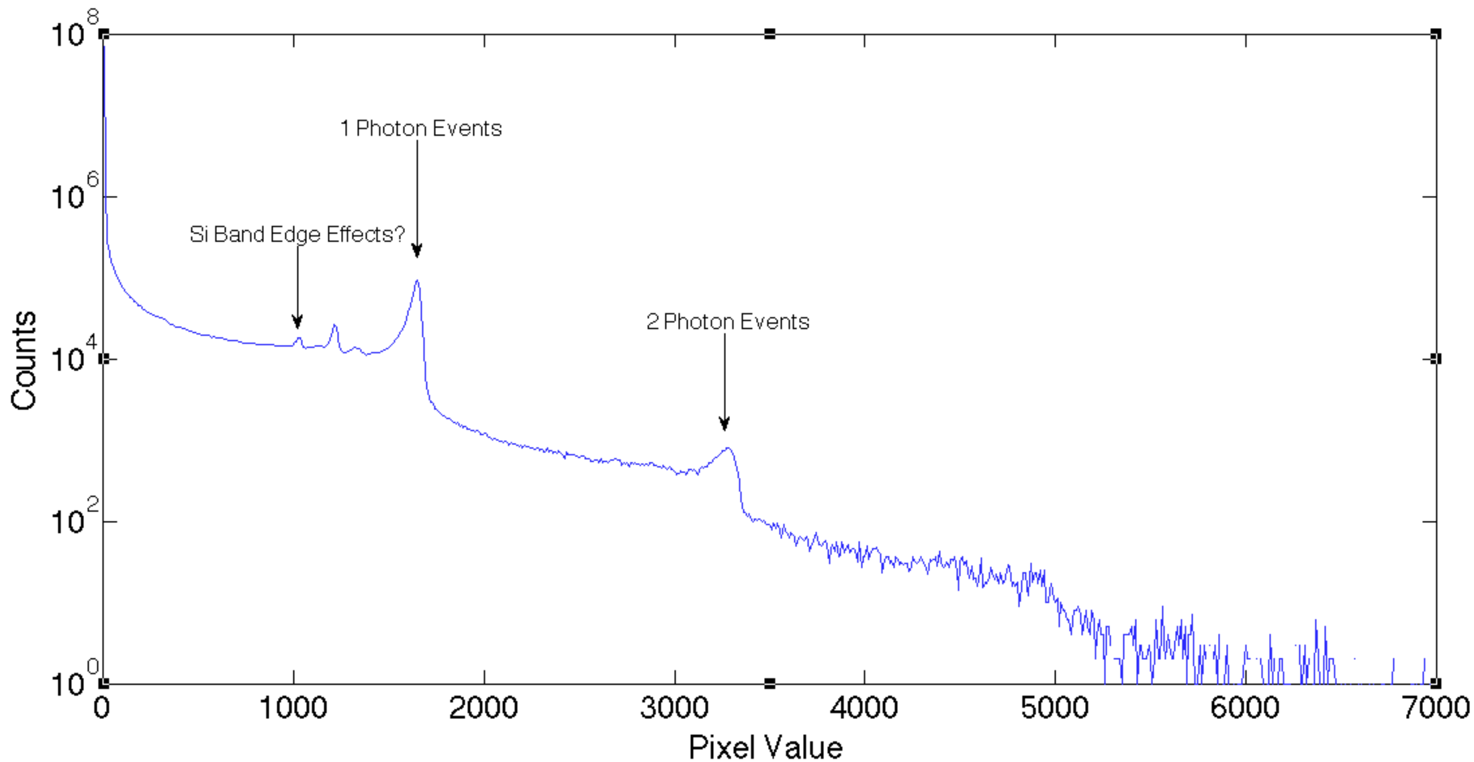
Run 87 (Au-NPs, 2 shots/frame)
V2
Frame
0
20
40
60
80
100
120
0
50
100
150
200
250

But they have a predictable 1/p relationship…



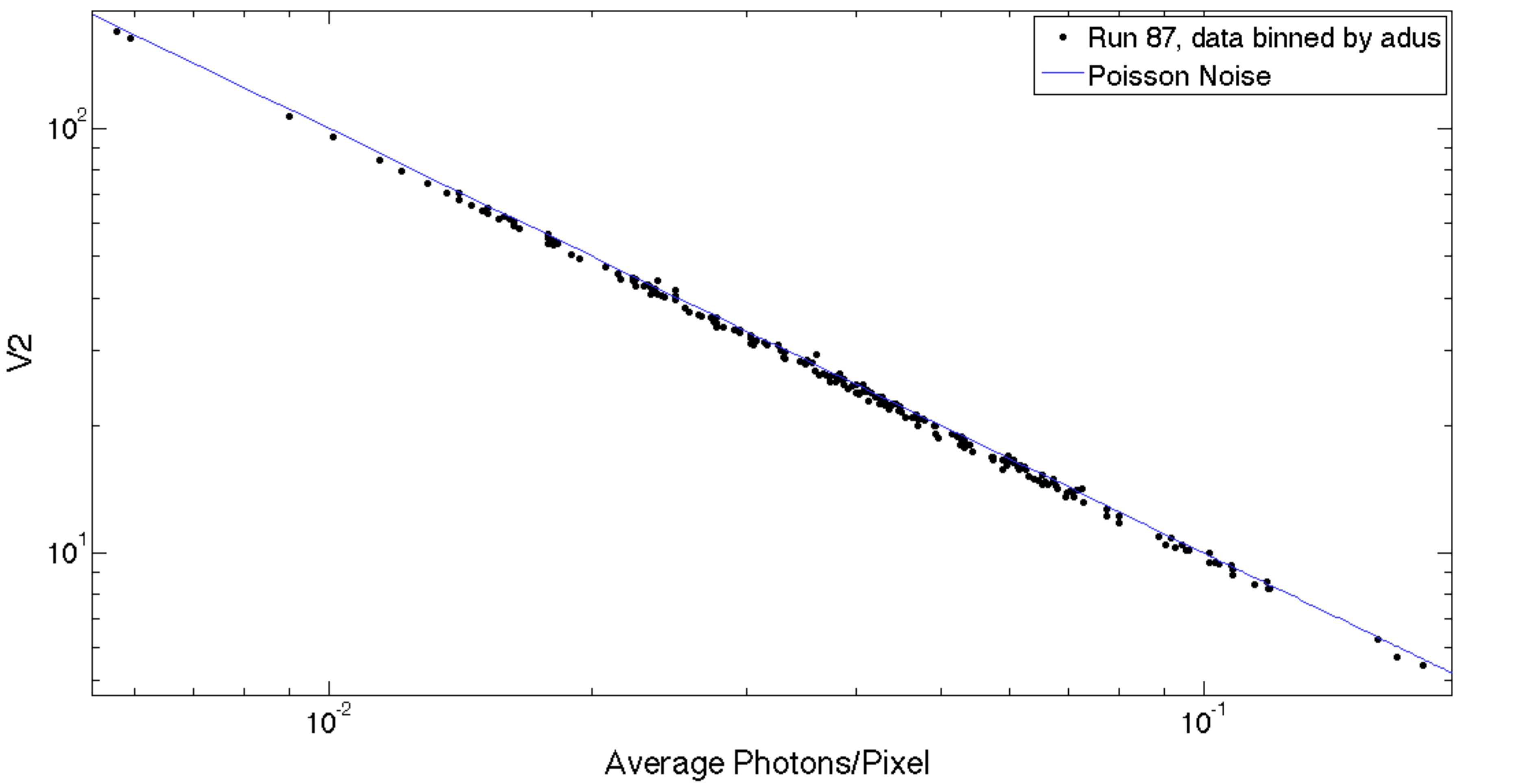
What accounts for the constant offset?

- A true Poisson distribution is a discrete distribution with point-masses at 0, 1, 2 photons, etc.
- A histogram of pixel values is continuous, and the intermediate values lower the variance.

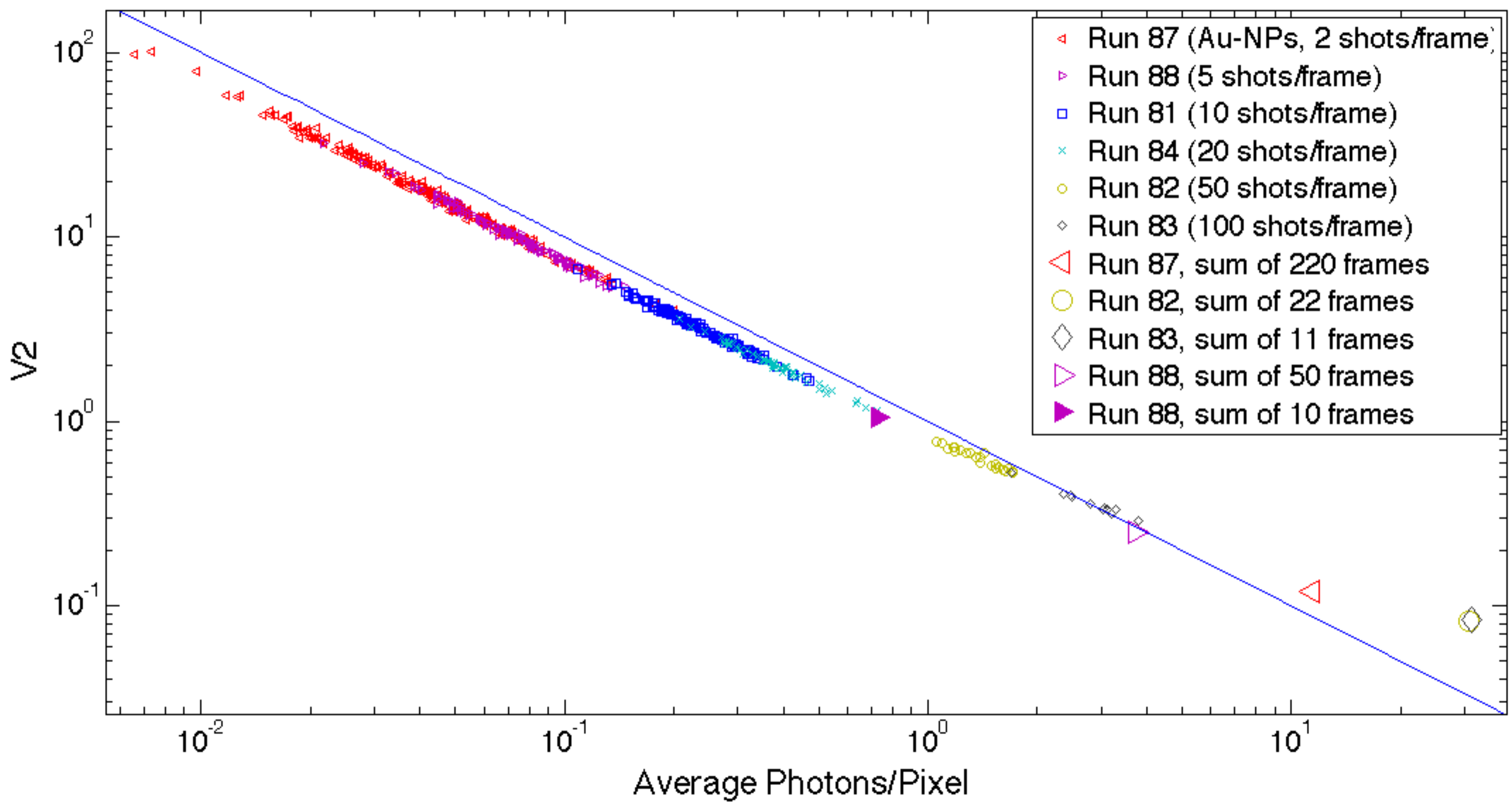


(Run 81, Au-NPs, 10 shots/frame. Histogram of full-frame images.)

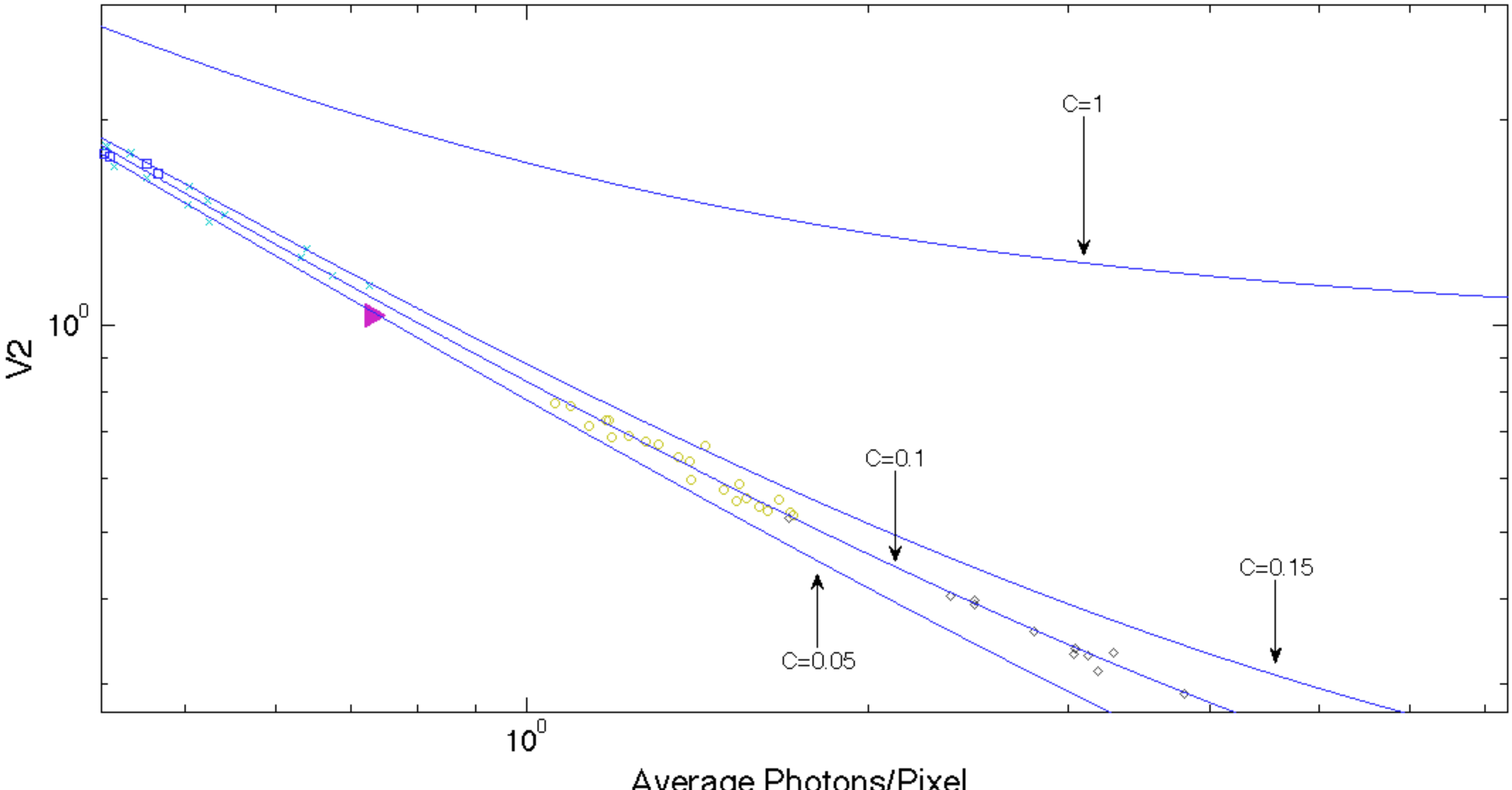
So if we bin the data into multiples of the adu, the offset should disappear:



As photons/pixel increases, one would expect V2 to level off to some value between 0 and 1…

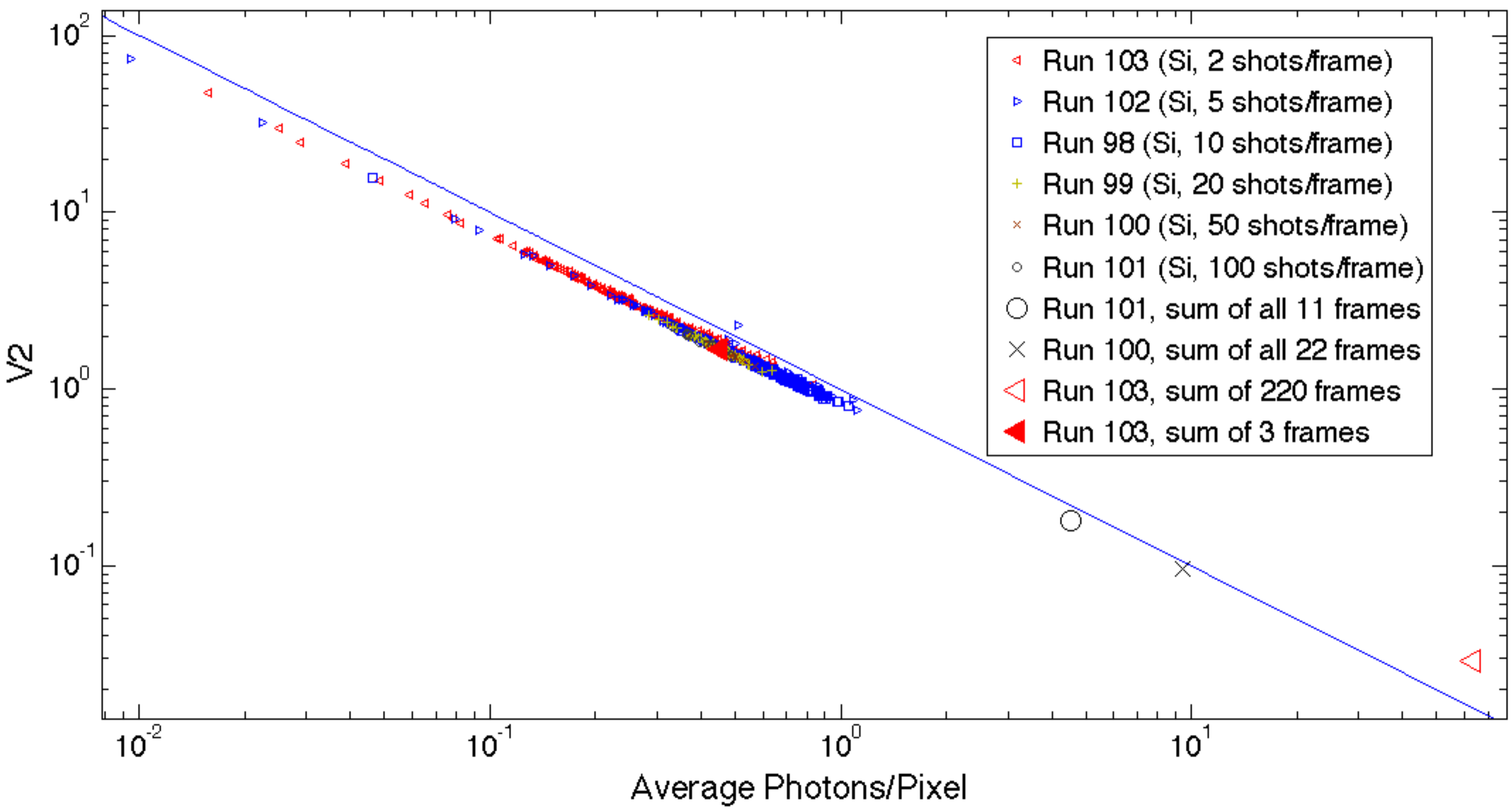


It appears to do so for the Au-NPs, but it would only be consistent with a contrast of ~ 10%...

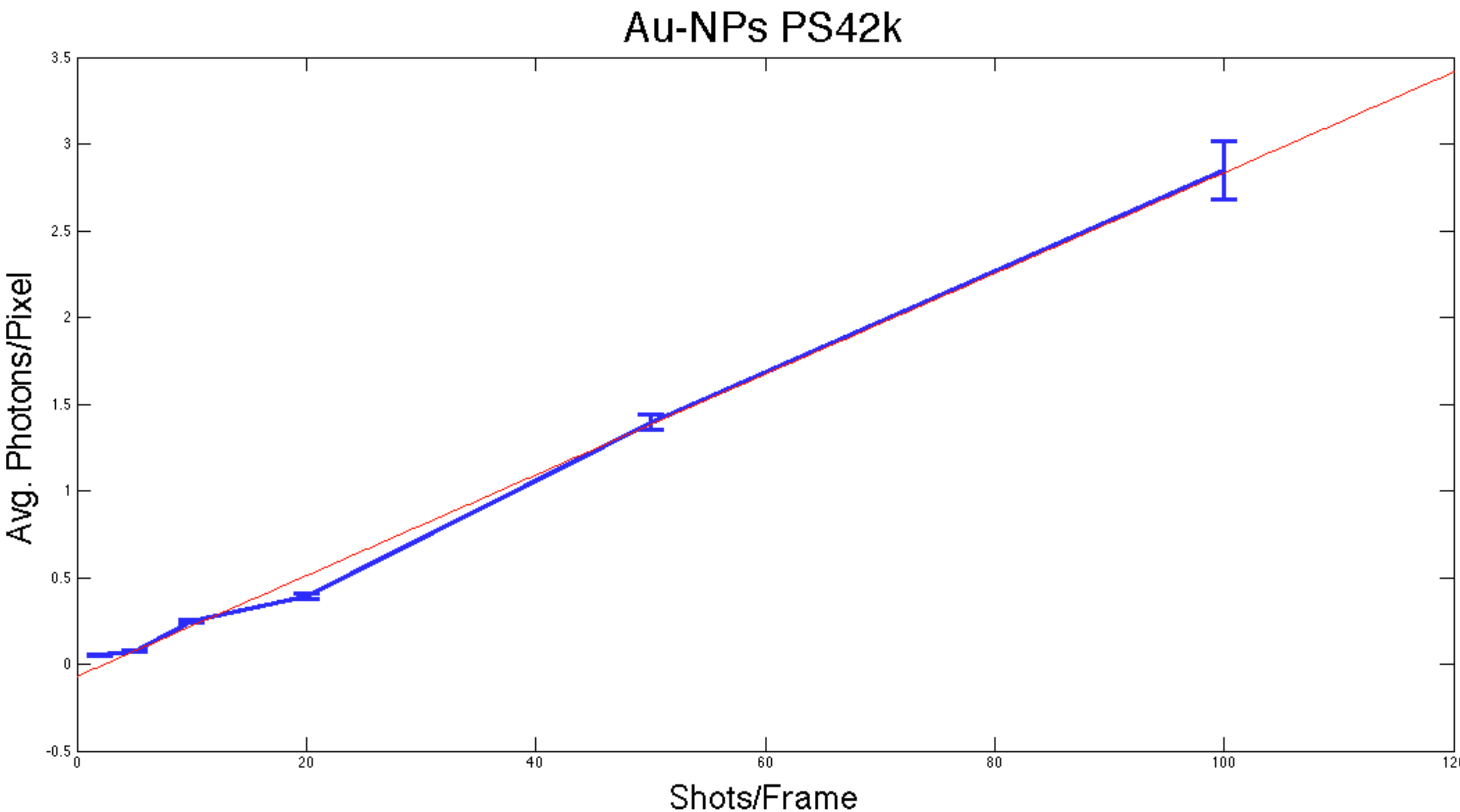


Formally(see Goodman), for static speckle overlaid with Poisson noise, the probability distribution should be a negative binomial distribution => V2=1/M+1/p, where M is the number of coherent modes, and p the average number of photoevents per pixel.

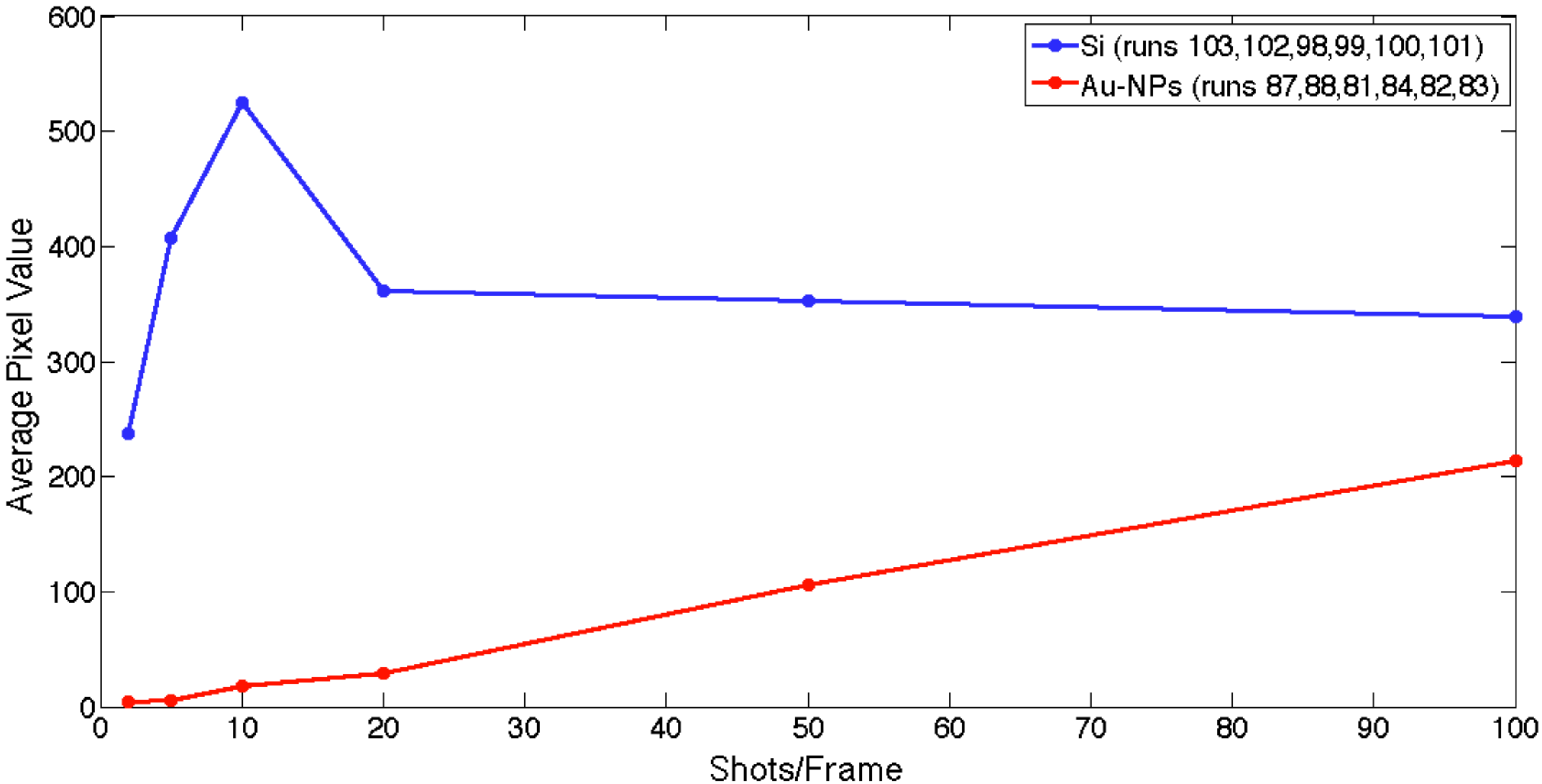
The Si sample appears less static than the Au-NP sample…



For the Au-NP sample, Intensity is linear in shots/frame.



But the Si sample shows strange dependence of intensity on shots/frame.

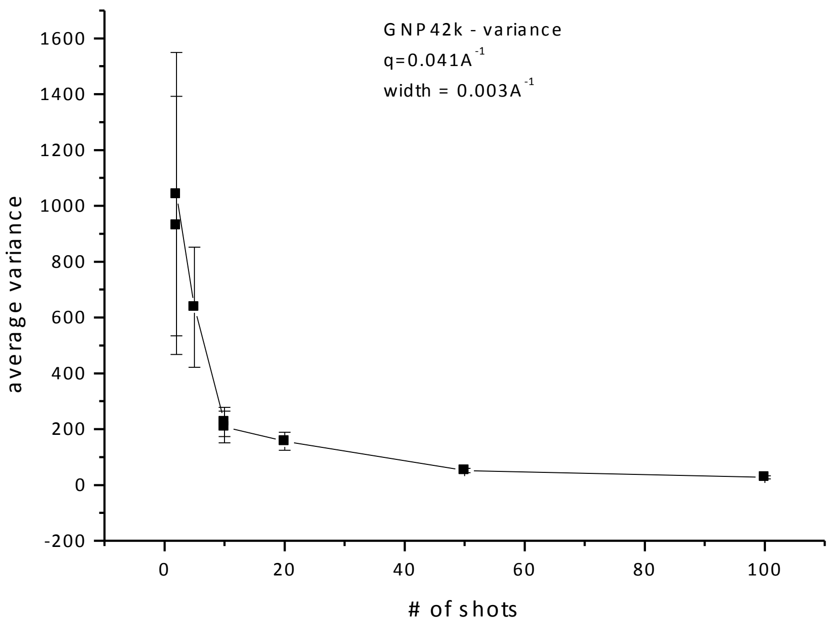


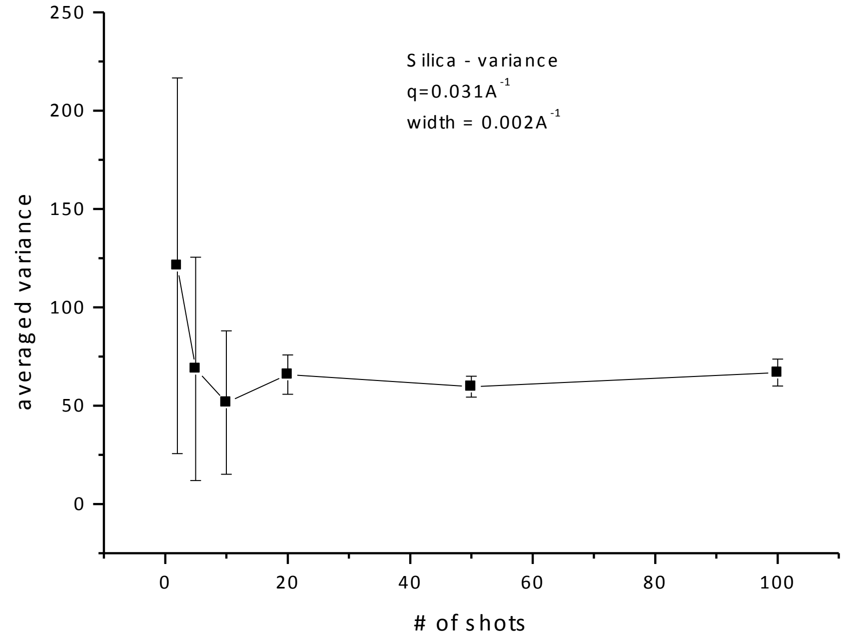
(Note: these values are for full frame images, but the same trend appears for all Q.)

Dynamics in the Si sample?

- Total intensity is flat with increasing shots/frame for the Si sample.
- Since Poisson noise is the main contribution to V2 in the low-photon regime, V2 is also flat with increasing shots/frame.
- Therefore, *plots of V2 vs. shots/frame are very misleading*, and would lead one to conclude that the Si sample does indeed appear static.

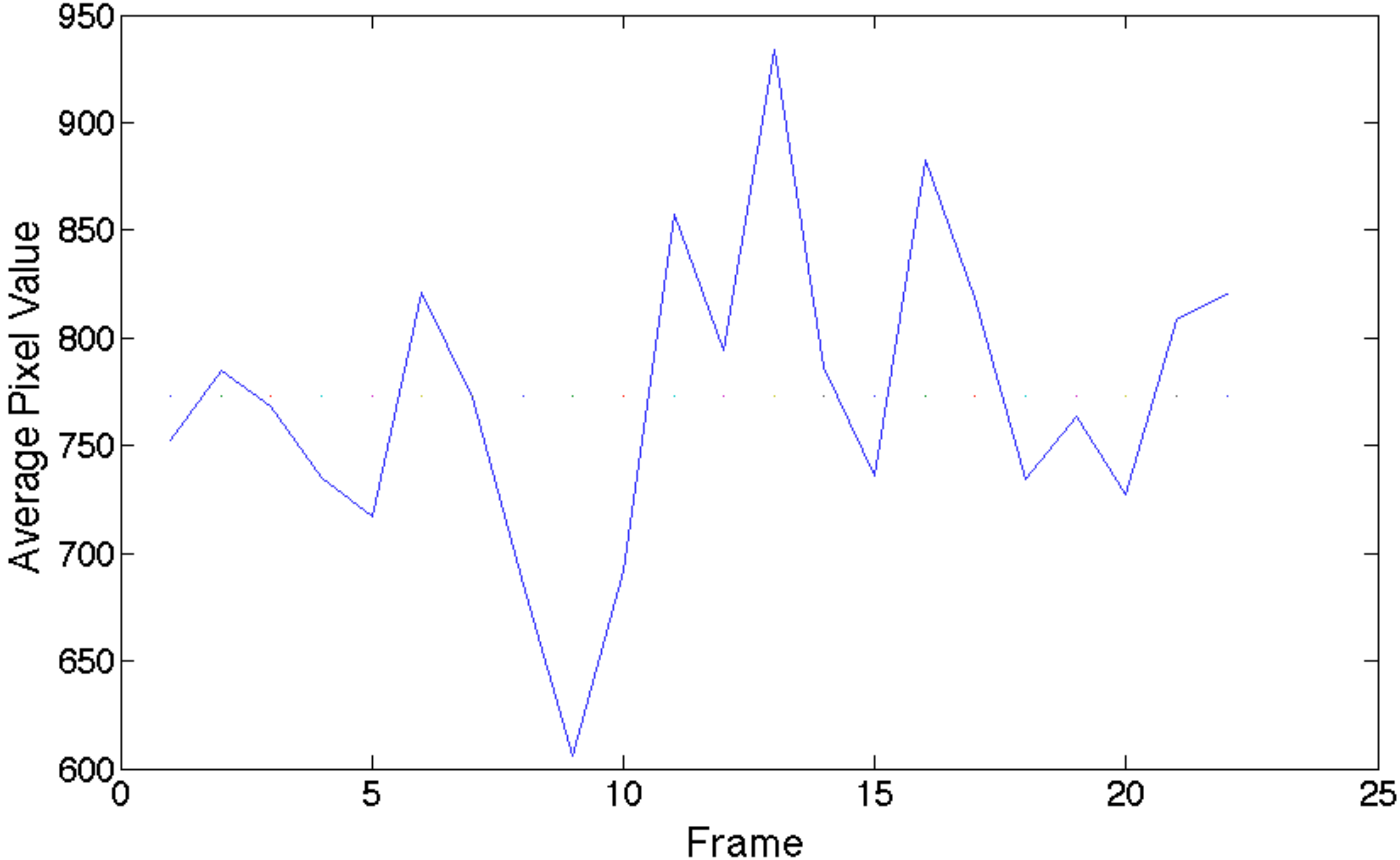
This unusual dependence of intensity on shots/frame completely explains why these plots differ:





(Images from Jerome Carnis)

What causes this behavior? Whatever it is, it does not lead to a trend in intensity across frames. (Run 100: Si, 50 shots/frame)



V2 & dynamics (SVS)

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- If sample dynamics are the cause, V2 is related to them in an analytic way:

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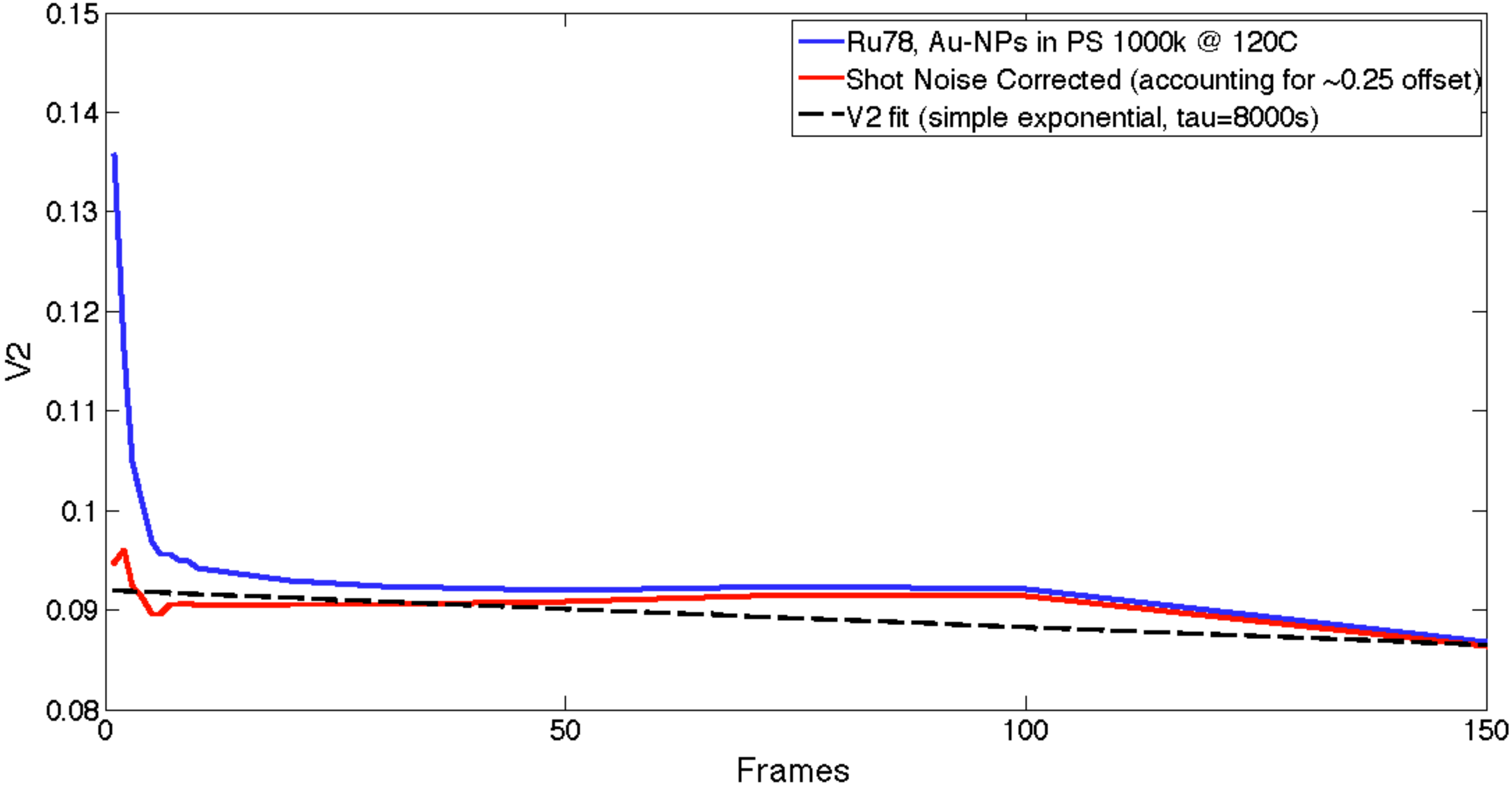
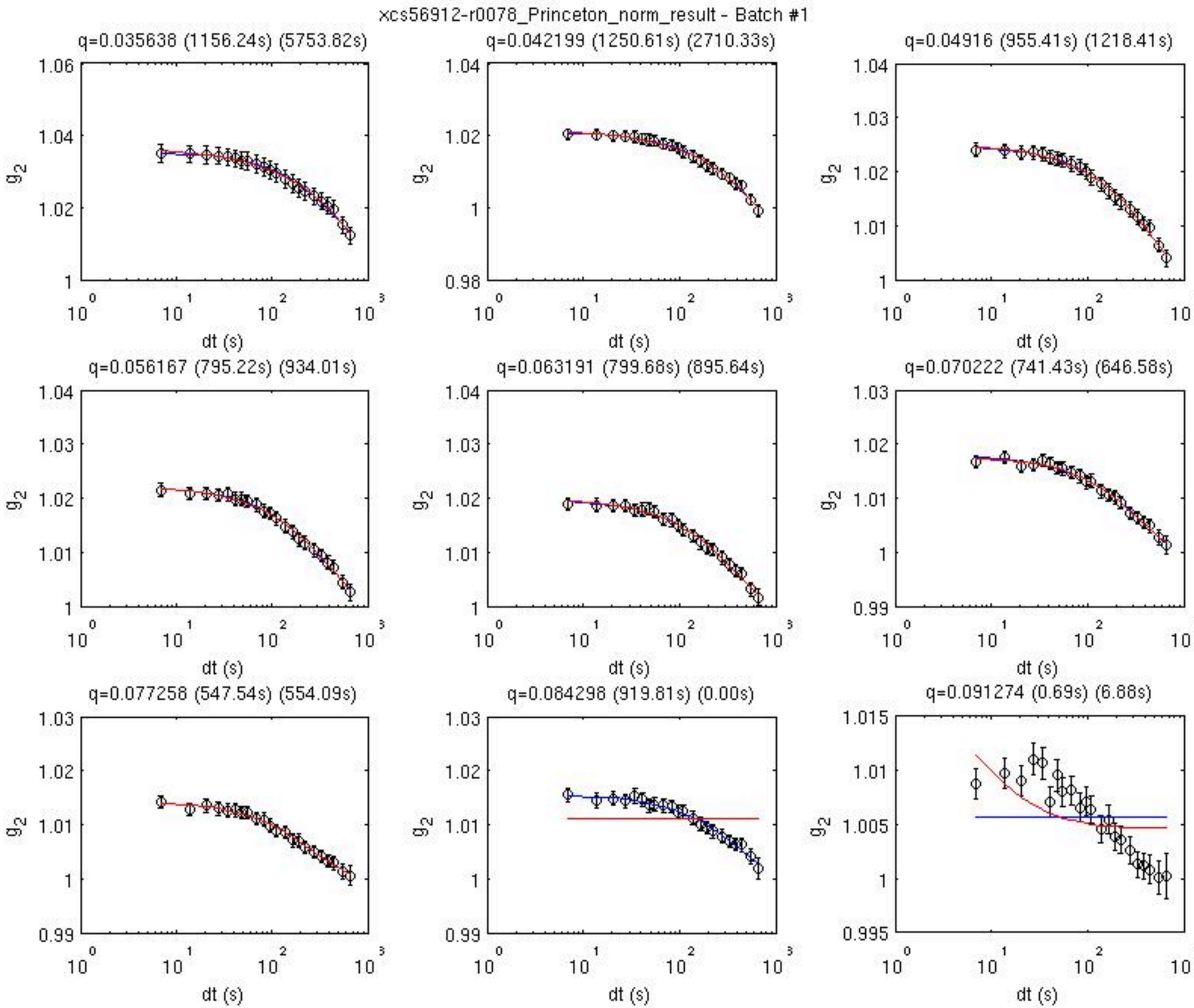
- For example,

$$g_1(\tau) = e^{-\Gamma\tau} => V_2 = \frac{e^{-2\Gamma\tau} - 1 + 2\Gamma\tau}{2(\Gamma\tau)^2}$$

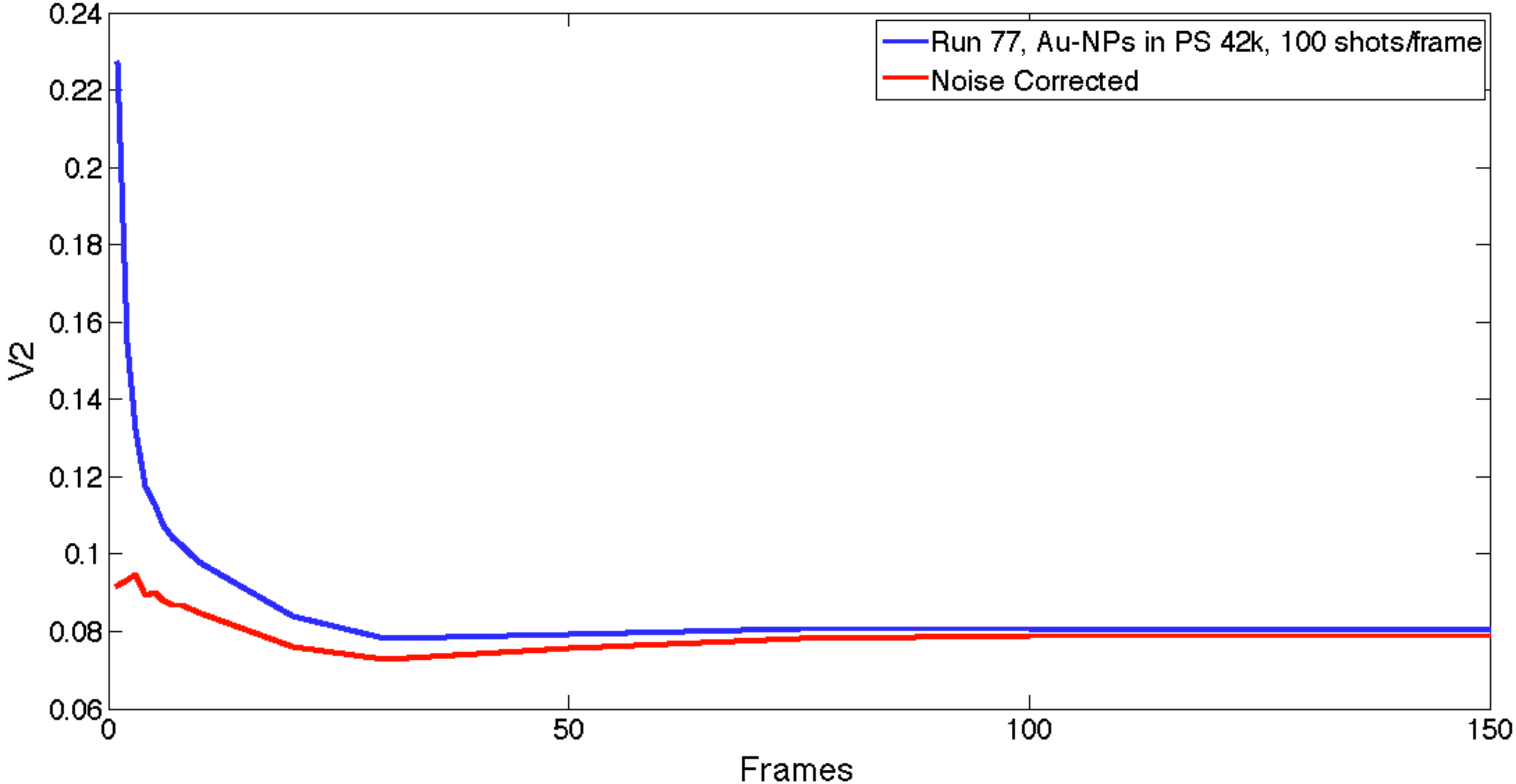
(Bandyopadhyay, et. al.)

V2 vs. frames merged for some longer runs (all 100 shots/frame)

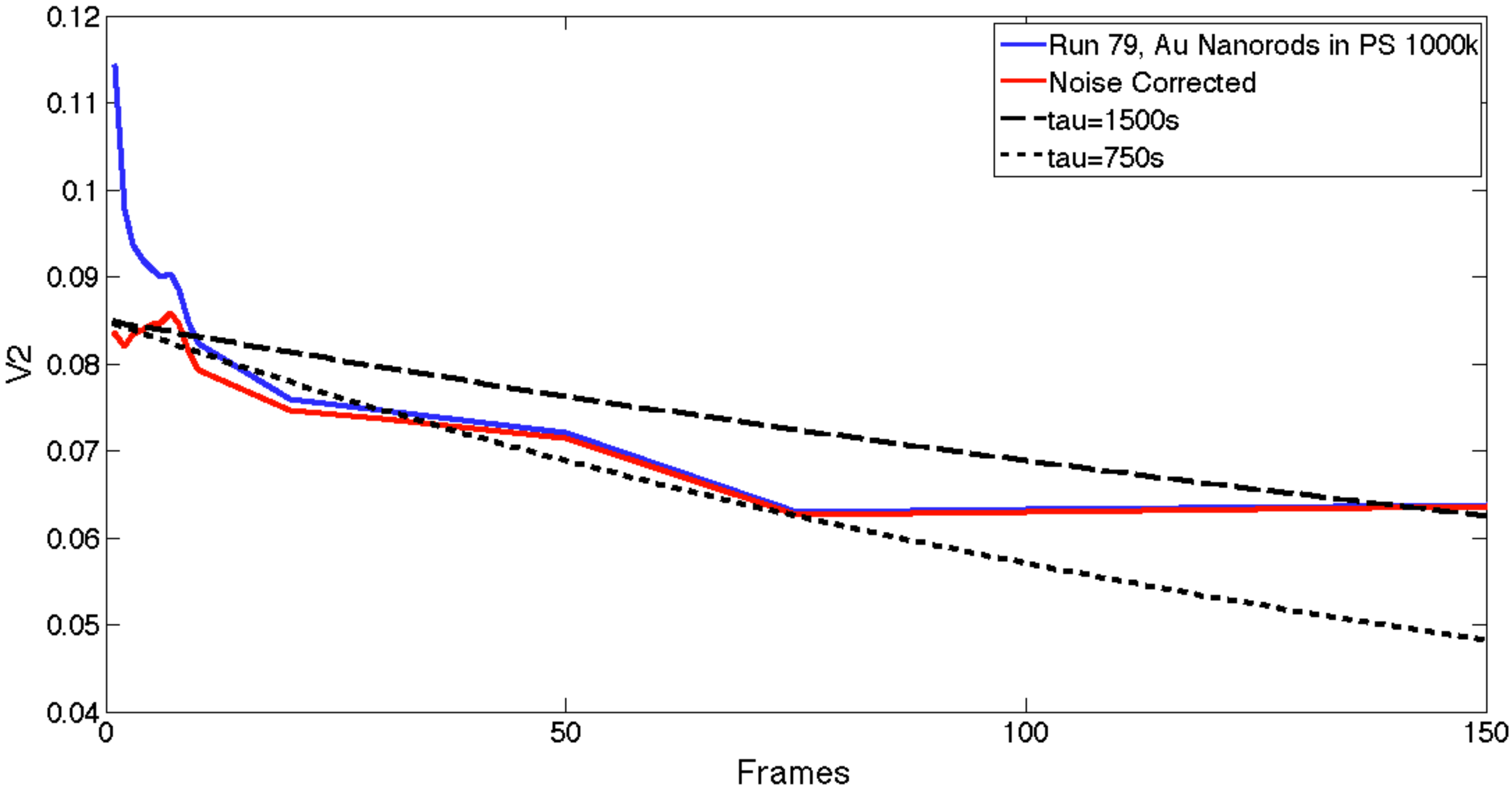


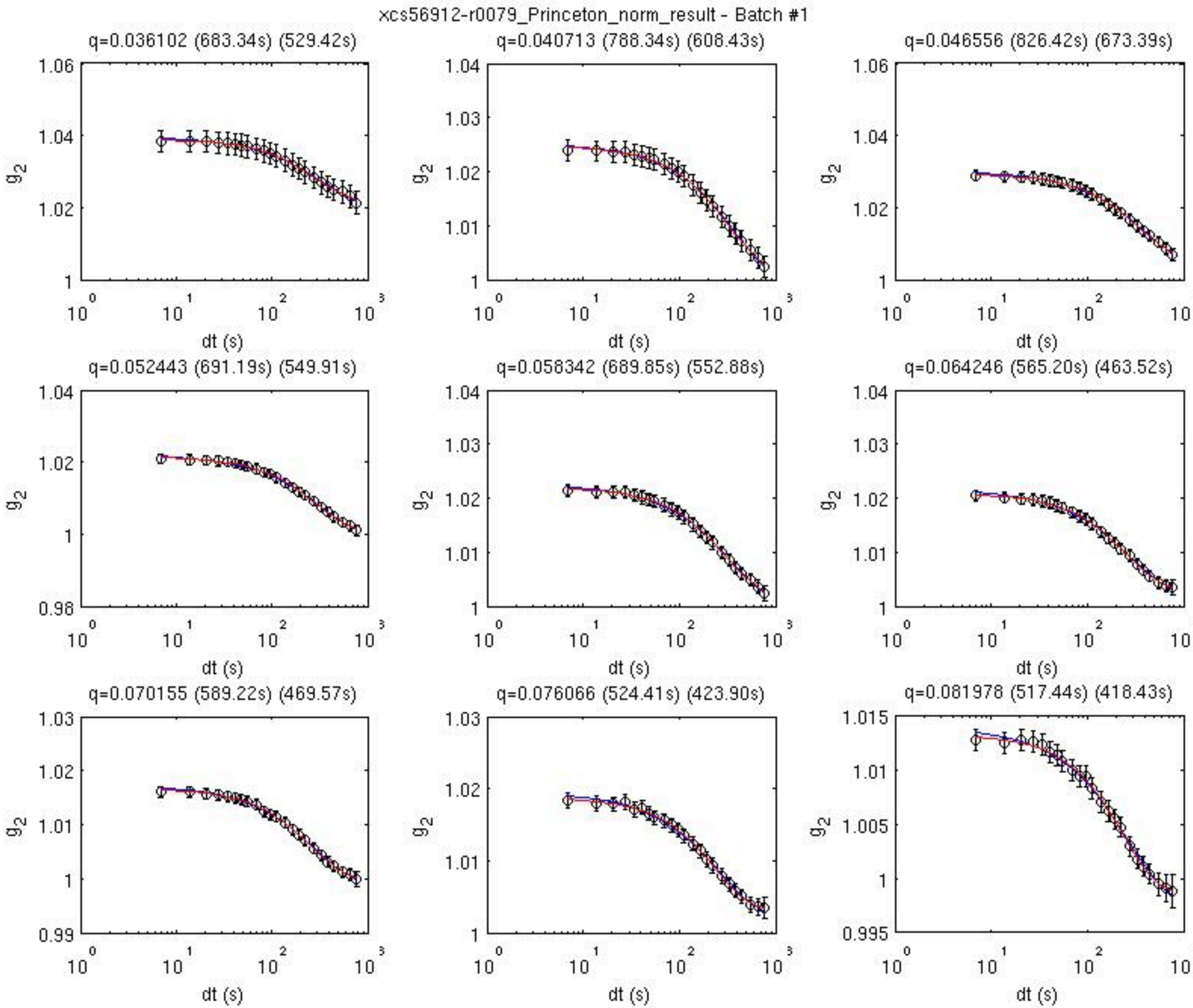

xcs56912-r0078_Princeton_norm_result - Batch #1
q=0.035638 (1156.24s) (5753.82s)
q=0.042199 (1250.61s) (2710.33s)
q=0.04916 (955.41s) (1218.41s)
q=0.056167 (795.22s) (934.01s)
q=0.063191 (799.68s) (895.64s)
q=0.070222 (741.43s) (646.58s)
q=0.077258 (547.54s) (554.09s)
q=0.084298 (919.81s) (0.00s)
q=0.091274 (0.69s) (6.88s)
g_2
dt (s)

Some runs show V2 rising after initial fall-off:



None really have a nice shape consistent with theory:



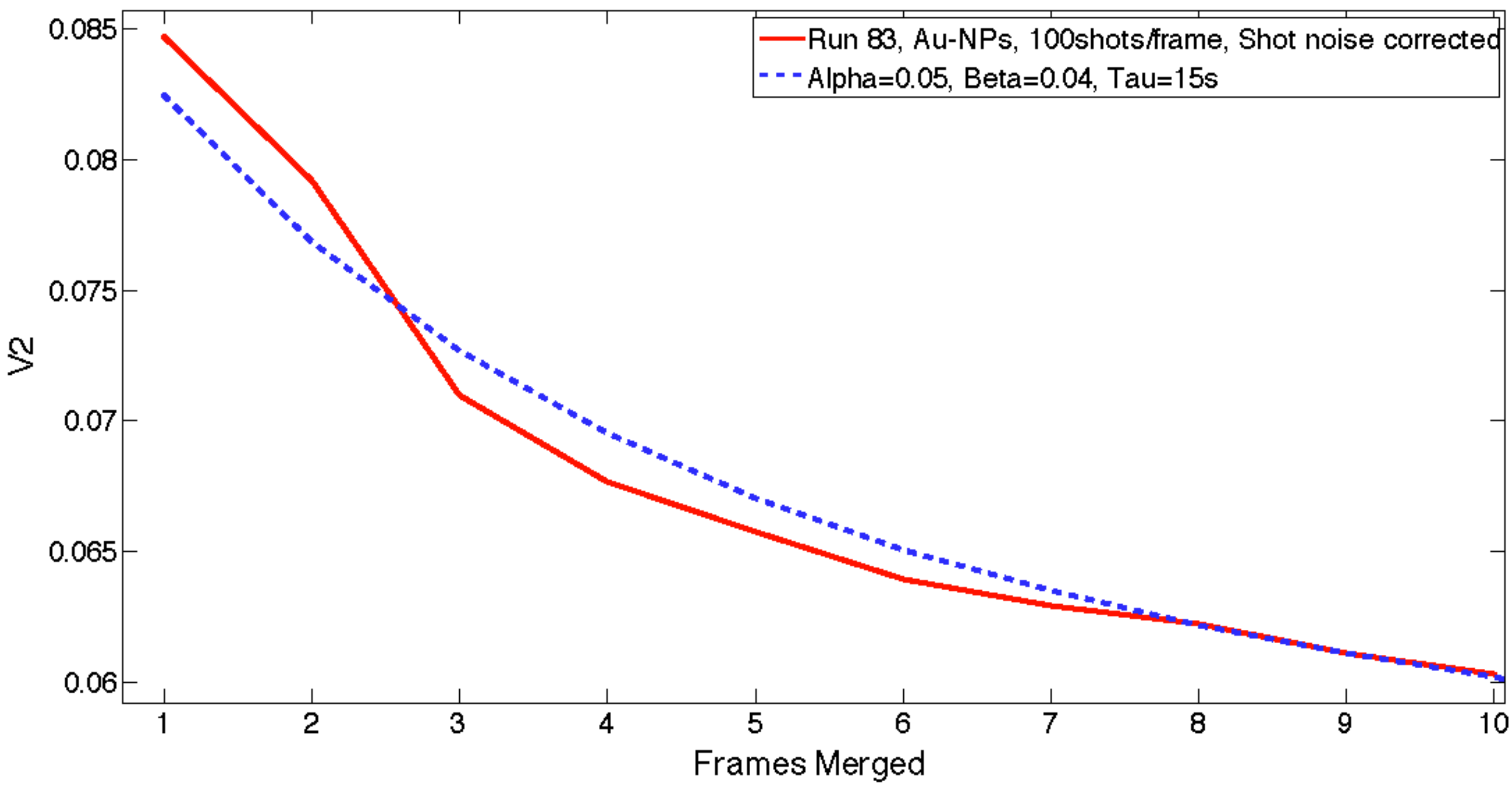

xcs56912-r0079_Princeton_norm_result - Batch #1
q=0.036102 (683.34s) (529.42s)
q=0.040713 (788.34s) (608.43s)
q=0.046556 (826.42s) (673.39s)
q=0.052443 (691.19s) (549.91s)
q=0.058342 (689.85s) (552.88s)
q=0.064246 (565.20s) (463.52s)
q=0.070155 (589.22s) (469.57s)
q=0.076066 (524.41s) (423.90s)
q=0.081978 (517.44s) (418.43s)
g_2
dt (s)

Rapid initial fall-off, persistently high V2

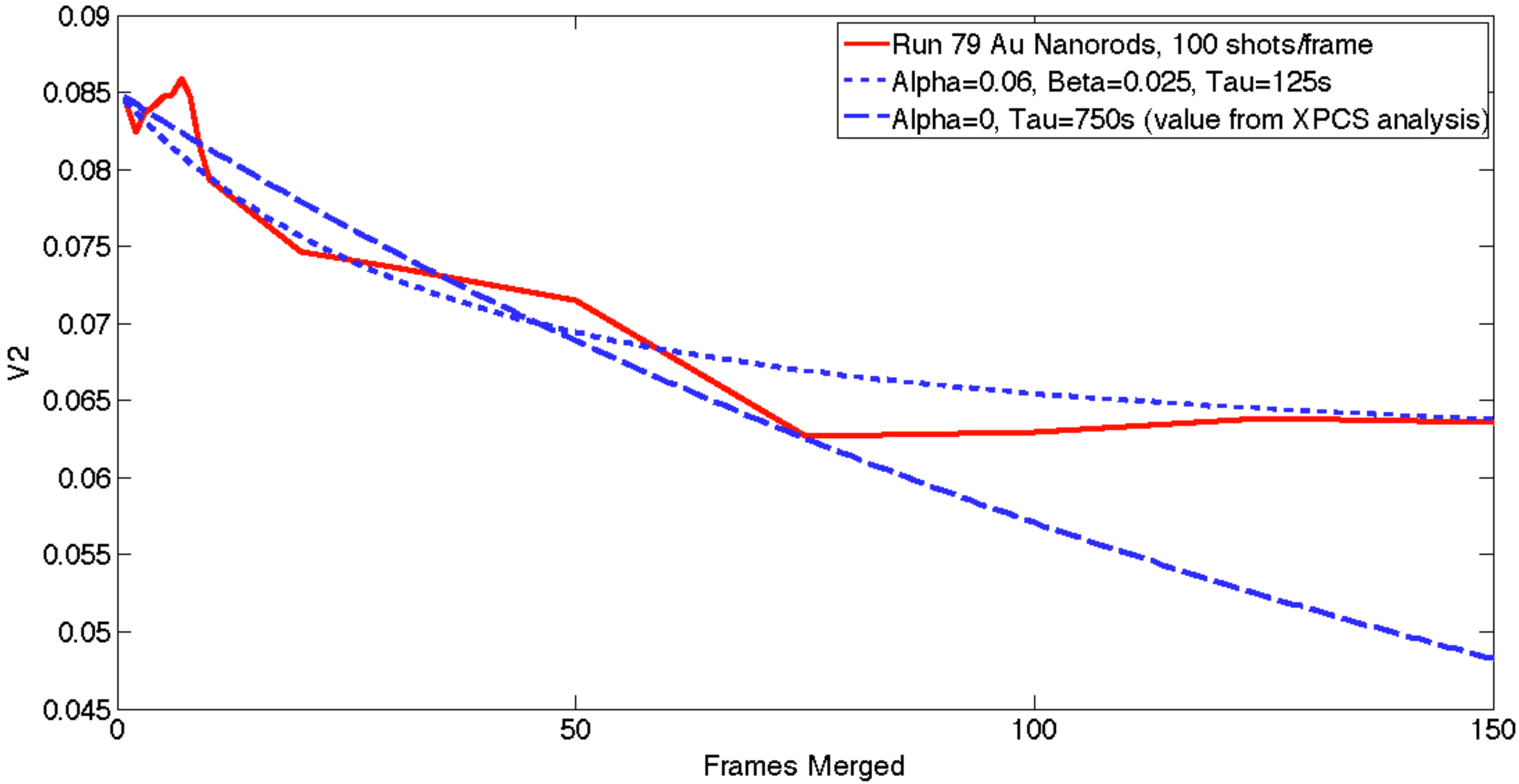
- Shot noise explains the fast initial fall-off.
- A “static” contribution to the speckle would explain why V2 levels off around at 5-10%.
- This could be due to truly static speckle (from lenses, for example) or an incomplete, long-term relaxation.
- In this case, one would expect V2 to have the form:

$$V_2 = \alpha + \beta \frac{e^{-2\Gamma\tau} - 1 + 2\Gamma\tau}{2(\Gamma\tau)^2}$$

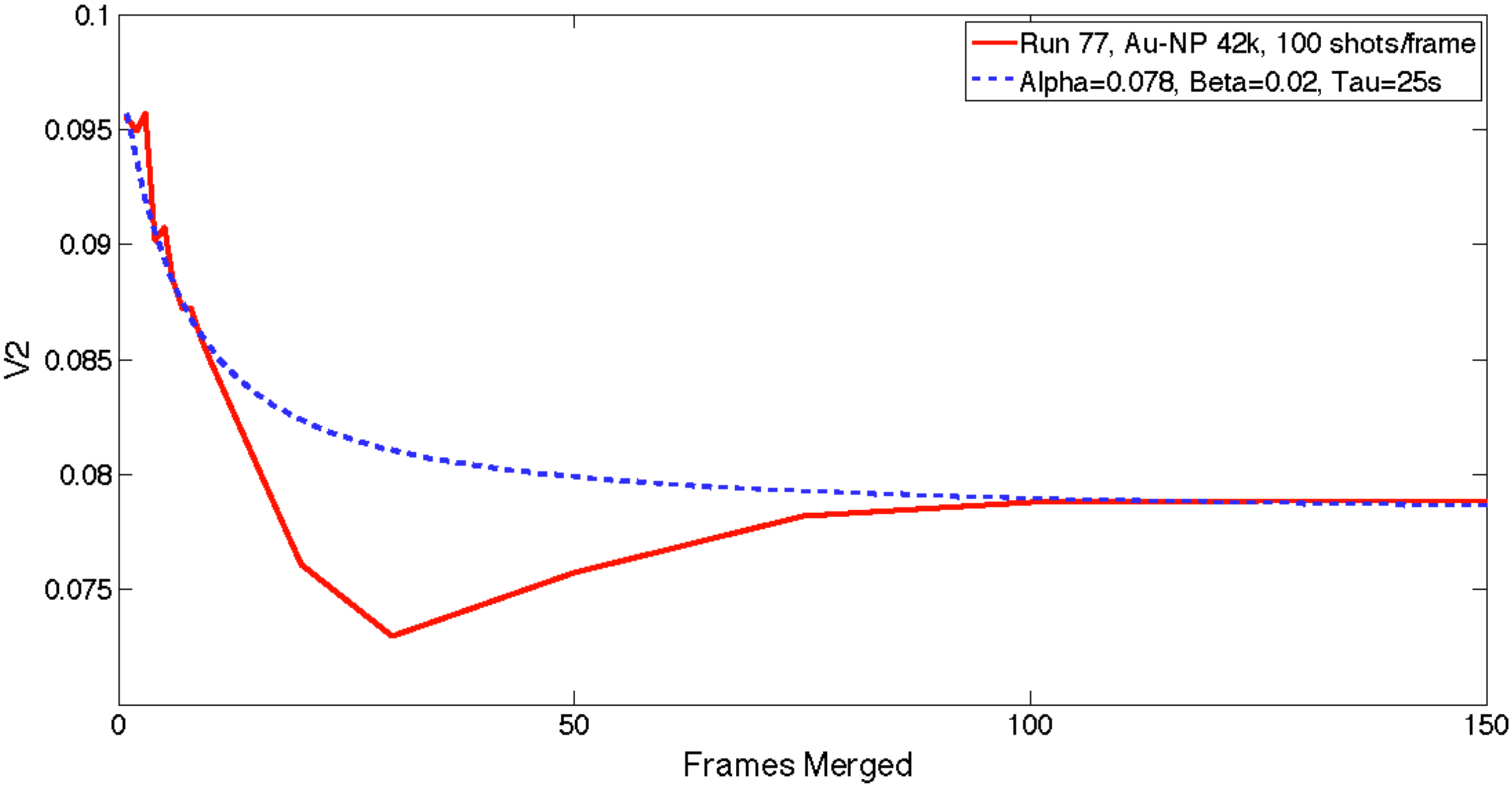
This seems to fit the data best.



Comparison to V2 one would expect from XPCS analysis



Some runs exhibit strange behavior



Collapsing Foam in Shpyrko Laser Lab